

Phenol, 2-methyl-5-(1-methylethyl)-

Other names:	1-Hydroxy-2-methyl-5-isopropylbenzene 2-Hydroxy-p-cymene 2-METHYL-5-ISOPROPYLPHENOL 2-Methyl-5-(1-methylethyl)phenol 2-p-Cymenol 3-Isopropyl-6-methylphenol 5-ISOPROPYL-2-METHYLPHENOL 5-Isopropyl-o-cresol 6-methyl-3-isopropylphenol Antioxine Carvacrol ISOTHYMOL Isopropyl-o-cresol Karvakrol NSC 6188 Oxycymol Phenol, 3-isopropyl-6-methyl- Phenol, 5-isopropyl-2-methyl- o-Cresol, 5-isopropyl- o-Thymol p-Cymen-2-ol p-Cymene, 2-hydroxy-
Inchi:	InChI=1S/C10H14O/c1-7(2)9-5-4-8(3)10(11)6-9/h4-7,11H,1-3H3
InchiKey:	RECUKUPTGUEGMW-UHFFFAOYSA-N
Formula:	C10H14O
SMILES:	<chem>Cc1ccc(C(C)C)cc1O</chem>
Mol. weight [g/mol]:	150.22
CAS:	499-75-2

Physical Properties

Property code	Value	Unit	Source
chl	-5650.00 ± 10.00	kJ/mol	NIST Webbook
chl	-5665.00	kJ/mol	NIST Webbook
gf	-20.96	kJ/mol	Joback Method
hf	-194.20	kJ/mol	NIST Webbook
hfl	-270.00	kJ/mol	NIST Webbook

hfus	17.57		kJ/mol	Joback Method
hvac	59.00 ± 3.00		kJ/mol	NIST Webbook
hvac	75.80		kJ/mol	NIST Webbook
hvac	77.74		kJ/mol	NIST Webbook
hvac	68.20		kJ/mol	NIST Webbook
log10ws	-2.08			Estimated Solubility Method
log10ws	-2.08			Aqueous Solubility Prediction Method
logp	2.824			Crippen Method
mccol	133.870		ml/mol	McGowan Method
pc	3439.94		kPa	Joback Method
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ripol	2239.00	NIST Webbook
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ripol	2239.00		NIST Webbook
ripol	2246.00		NIST Webbook
ripol	2239.00		NIST Webbook
ripol	2240.00		NIST Webbook
ripol	2199.00		NIST Webbook
ripol	2240.00		NIST Webbook
ripol	2239.00		NIST Webbook
tb	510.25 ± 3.00	K	NIST Webbook
tb	509.70	K	NIST Webbook
tb	510.90	K	NIST Webbook
tb	510.25 ± 3.00	K	NIST Webbook
tb	510.25 ± 3.00	K	NIST Webbook
tb	509.15 ± 3.00	K	NIST Webbook
tb	510.45 ± 0.30	K	NIST Webbook
tb	509.15 ± 4.00	K	NIST Webbook
tc	764.51	K	Joback Method
tf	274.65	K	Aqueous Solubility Prediction Method
tf	276.65 ± 2.00	K	NIST Webbook
tf	276.65 ± 2.00	K	NIST Webbook
tf	273.65 ± 3.00	K	NIST Webbook
vc	0.448	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	311.65	J/mol×K	540.04	Joback Method
cpg	325.50	J/mol×K	577.45	Joback Method
cpg	338.45	J/mol×K	614.86	Joback Method
cpg	350.56	J/mol×K	652.28	Joback Method
cpg	361.90	J/mol×K	689.69	Joback Method
cpg	372.56	J/mol×K	727.10	Joback Method

cpg	382.61	J/molxK	764.51	Joback Method
dvisc	0.0012767	Paxs	371.77	Joback Method
dvisc	0.0035167	Paxs	338.12	Joback Method
dvisc	0.0005484	Paxs	405.43	Joback Method
dvisc	0.0002681	Paxs	439.08	Joback Method
dvisc	0.0001452	Paxs	472.73	Joback Method
dvisc	0.0000853	Paxs	506.39	Joback Method
dvisc	0.0000535	Paxs	540.04	Joback Method
hvapt	56.50	kJ/mol	426.50	NIST Webbook
hvapt	59.40	kJ/mol	449.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.54478e+01
Coeff. B	-4.62610e+03
Coeff. C	-8.29720e+01
Temperature range (K), min.	388.12
Temperature range (K), max.	539.36

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/T + C \cdot \ln(T) + D \cdot T^2$
Coeff. A	1.40397e+01
Coeff. B	-6.60997e+03
Coeff. C	5.77820e-01
Coeff. D	-2.68503e-07
Temperature range (K), min.	343.15
Temperature range (K), max.	510.15

Sources

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Aqueous Solubility Prediction Method: <http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx>
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NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C499752&Units=SI>
KDB Vapor Pressure Data: <https://www.chemic.org/research/kdb/hcprop/showprop.php?cmpid=883>
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Legend

chl: Standard liquid enthalpy of combustion
cp_g: Ideal gas heat capacity
d_{visc}: Dynamic viscosity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions
h_{fl}: Liquid phase enthalpy of formation at standard conditions
h_{fus}: Enthalpy of fusion at standard conditions
h_{vap}: Enthalpy of vaporization at standard conditions
h_{vapt}: Enthalpy of vaporization at a given temperature
log₁₀ws: Log₁₀ of Water solubility in mol/l
log_p: Octanol/Water partition coefficient
mc_{vol}: McGowan's characteristic volume
pc: Critical Pressure
p_{vap}: Vapor pressure
ri_{npol}: Non-polar retention indices
ri_{pol}: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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